Supporting Information for "First-principles investigation of high capacity, rechargeable CF_x cathode batteries based on graphdiyne and "holey" graphene carbon allotropes"

Quinn T. Campbell[a], Nirajan Paudel[b], Krishna Acharya[b], Bryan R. Wygant[c], Igor Vasiliev[b], T. N. Lambert[a]

[a] Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM, USA
[b] Department of Physics, New Mexico State University, Las Cruces, NM, USA
[c] Nanoscale Sciences Department, Sandia National Laboratories, Albuquerque, NM, USA

Section S.1 Nonequilibrium structures considered

Throughout the main manuscript, we display the structure of equilibrium structures in the main figures. We have, however, tested several alternative structures which turned out to be unstable to reach these structures. We here display a number of these structures along with their energies to demonstrate our attempt at finding local minima.

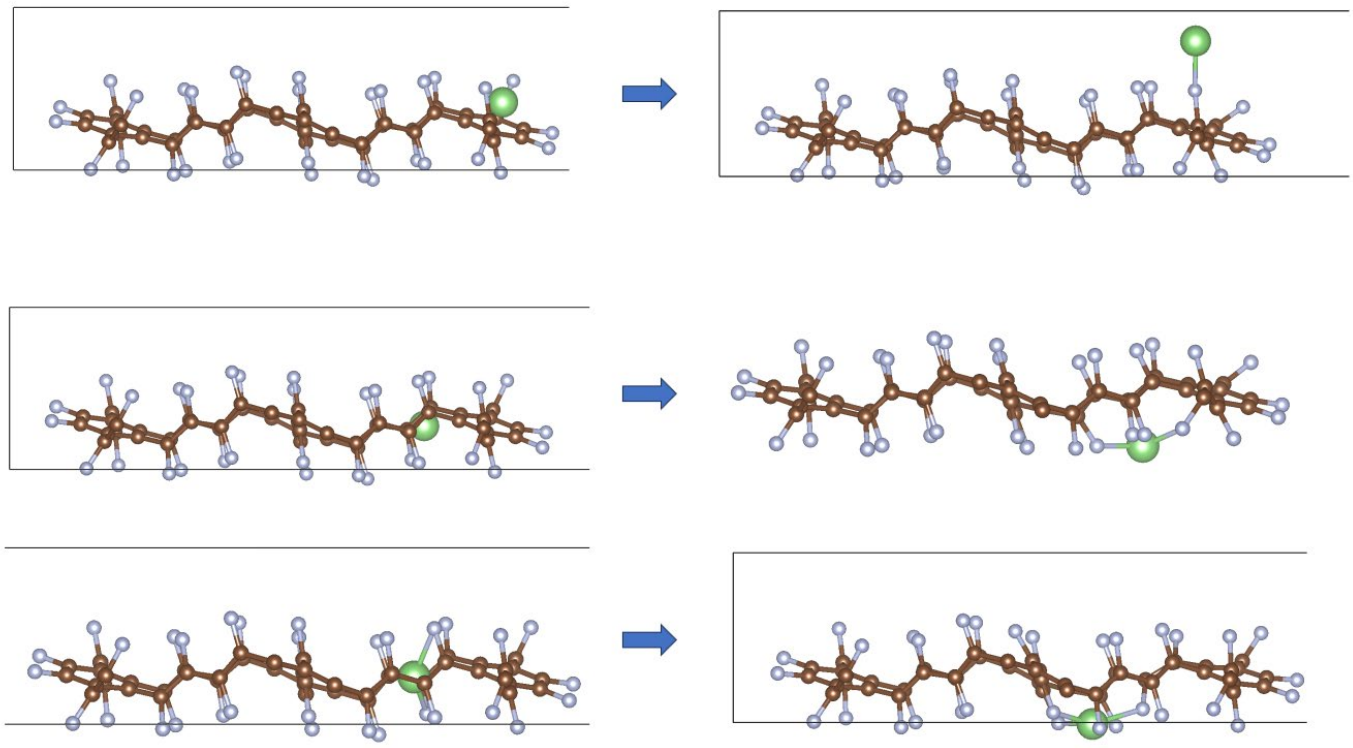

Fig. S1 Diagrams of the structures corresponding to attempting to attach a Li atom to the C atoms of the graphdiyne. Li consistently moves toward bonding with F after geometry optimization.

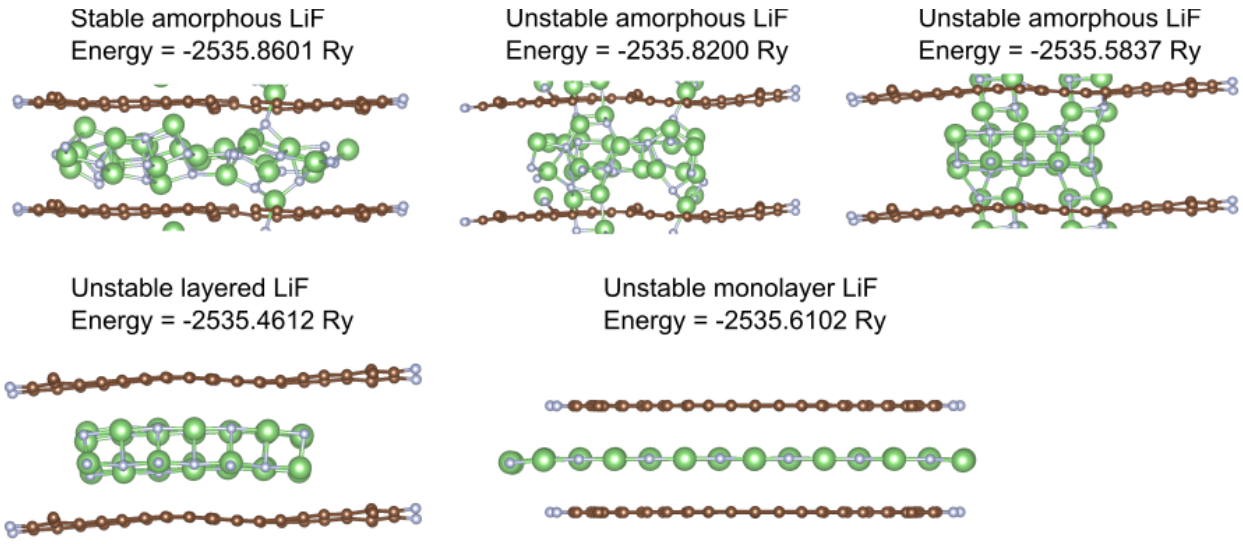

Fig. S2 Diagrams of the non-equilibrium structures tested for graphdiyne with LiF. We find amorphous LiF structures to be consistently favored.

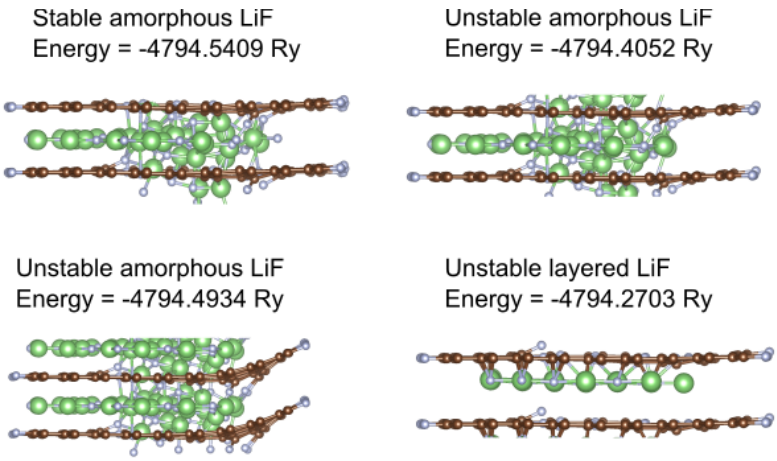

Fig. S3 Diagrams of the non-equilibrium structures tested for holey graphene with LiF. We find amorphous LiF structures to be consistently favored.